## MCNP Estimate of the Sampled Volume in a Non-Destructive In Situ Soil Carbon Analysis

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#### **Abstract**

Global warming, promoted by anthropogenic CO<sub>2</sub> emission into the atmosphere, is partially mitigated by the photosynthesis processes of the terrestrial echo systems that act as atmospheric CO<sub>2</sub> scrubbers and sequester carbon in soil. Switching from till to no till soils management practices in agriculture further augments this process. Carbon sequestration is also advanced by putting forward a carbon "credit" system whereby these can be traded between CO<sub>2</sub> producers and sequesters. Implementation of carbon "credit" trade will be further promulgated by recent development of a non-destructive *in situ* carbon monitoring system based on inelastic neutron scattering (INS). Volumes and depth distributions defined by the 0.1, 1.0, 10, 50, and 90 percent neutron isofluxes, from a point source located at either 5 or 30 cm above the surface, were estimated using Mont Carlo calculations.

**Key Words:** Soil, carbon sequestration, neutrons, MCNP

#### Introduction

A central theme of research on the terrestrial carbon sink over the last decade is the hypothesis that there is a large terrestrial sink for the atmospheric CO<sub>2</sub> [Sarmiento and Wofsy, 1999]. The magnitude of this sink was estimated to be on the order of 1.5  $\pm$  1.0 Gt C/yr for 1980-1989 [Schimel et al. 1996] and as having increased to > 2.5 Gt C/yr in the last decade, which is about 25% of the annual CO<sub>2</sub> emission into the atmosphere. Potential consequences of the steadily increase in the atmospheric emissions are partially mitigated by the photosynthesis processes in plants that remove CO<sub>2</sub> from the atmosphere and sequester in soil. Corollary benefits of carbon sequestration are increased soil fertility, reduction in erosion, and improved soil quality. Furthermore, under private emission trading strategy, what is evolving is that farmers would be able to sell carbon "credits" to CO<sub>2</sub> emitting industry. This market is estimated in US at about \$1-5 billions per year for the next 30-40 years [Rice, 2004]. These two issues; carbon sinks and trade with carbon "credits", require novel instrumentation that would enable a better understanding of the belowground carbon processes. At the same time, more importantly for the trade carbon "credit" system development, it will allow a direct quantitative measure of the belowground carbon stores in situ in a non-destructive manner over a single spot or alternatively over continuously scanned large areas.

Current method of quantifying carbon in soil by core sampling is slow, invasive, labor intensive, and, consequently, very limited in its utility. Two newly emerging methods to measure carbon in soil *in situ* are a Laser Induced Breakdown Spectroscopy (LIBS) [Cramers et al., 2001] and a near and mid infrared spectroscopy [McCarty et al., 2002]. However, these methods although presenting improvements over core sampling are destructive. In the first case, a small volume of about 50 micro-liters is vaporized and the resulting spectral emission is measured. In the second case, a sensor mounted on a tip of a shank ploughs through the soil at a set depth and

senses the carbon to a depth of few millimeters. A third method, based on inelastic neutron scattering (INS) and prompt measurement of characteristic gamma rays from carbon, has been demonstrated [Wielopolski et al., 2000 and Wielopolski et al., 2003]. The INS method is truly non-destructive can be used for repetitive measurements at exactly the same spot as well as for continuous scan over large areas. Fundamentals of the method and descriptions of its components can be found in [Csikai, 1987] and in [Nargolwalla and Przybylowicz, 1973], the INS system calibration and operation has been recently published by Wielopolski et al., [2004].

The large volumes, V, sampled by the INS method can be separated into two components, one, the irradiated volume by the fast neutrons,  $V_i$ , and , two, the intercept of that volume by the solid angle subtended by the gamma ray detection system. The overall sampled volume is critically important for proper assessment of the total carbon measured. The irradiated volumes  $V_i$  defined by the 0.1, 1.0, 10, 50, and 90 percent neutron isofluxes levels in the soil are estimated using Monte Carlo method and reported here.

#### Method

A Monte Carlo Neutron Photon (MCNP) probabilistic transport code employed in the present work [Breismeister, 1993], is one of several codes used for radiation transport calculations. These codes require input information that usually contain the geometrical configuration of the system being simulated, elemental soil composition, in our work we used O 55%, Si 35%, Al 7.2%, and Fe 2.6% by weight, and soil density, 1.45 g/cm³. In addition, each execution requires the number of histories, which is the number of neutrons that are followed from birth to death we used 10<sup>8</sup> histories. The neutron source was either an isotropic point source or a pencil beam emitting, in either case, 14 MeV monoenergetic neutrons. The geometry was simply placing the point source at 5 cm and 30 cm above the ground and calculating the neutron fluxes in the soil using F2 MCNP tallies, which score the neutron fluxes intercepting specified surfaces. The scoring cell was a soil cell 1cm in diameter and 1 cm thick.

## **Results**

The basic neutron flux distributions in soil from a monoenergetic 14 MeV neutron point source located at various distances above the ground are shown in Fig. 1. These fluxes represent neutron energy group from about 4.6 MeV, which is the threshold energy for inelastic neutron scattering in carbon, up to and including 14 MeV neutrons. The neutron energy spectra not shown here undergo elastic scattering and change with depth. The lines in Fig. 1 represent neutron fluxes,  $\phi$ , given by a simple model below

$$\phi = (1/4\pi) \exp(-1.45 * 0.02 * D) / (H+D)^2$$
 (1)

where: H is the height of the source above the ground and D is the depth below the surface. The constant 1.45 g/cc is the soil density and 0.02 represent an effective macroscopic neutron mass attenuation that at present was loosely determined to fit the MCNP calculated fluxes denoted in Fig. 1 by the various symbols. The neutron fluxes normalized to the flux at the surface, by multiplying  $\phi$  by H<sup>2</sup>, are shown in Fig. 2 demonstrate an improved irradiation uniformity in soil when source is elevated above the ground.

Since the point source above the ground has axial symmetry (symmetry around a normal from the point source to the ground) the model given in Eq. 1 was used to create three-

dimensional flux distributions in the soil. These for source positioning at H equals 5 and 30 cm are shown in Figs. 3 and 4, respectively. Note the x-axis in Figs. 3 and 4 have different scales. The corresponding isoflux contour lines at 0.1, 1.0, 10.0, 50.0 and 90.0 percent levels for source positioning at 5 and 30 cm are shown in Figs. 5 and 6, respectively. The resulting volumes and masses encompassed by these contour lines were calculated and are summarized in Table 1.

To understand better the mechanism of flattening of the neutron flux gradient with depth when the source distance above the ground is increased; first, the effect on the surface flux and, second, assuming a parallel beam the effect of the beam width on the depth flux distribution were simulated. Flattening of the lateral spread of the surface flux with increase in the source elevation is shown in Fig. 7. Varying the diameter of a parallel neutron beam increases the neutron flux at a given depth by increasing the in-scattering of neutrons into the monitoring point. These calculations are shown in Fig. 8 where the results were normalized twice at depth of 5 cm and to a beam diameter of 1.0 cm.

Variation of the neutron energy spectra with depth for 0 and 50 cm depth in soil are shown in Fig 9. Finally the relevance of this analysis is demonstrated in Fig 10 showing the increase in the net carbon signal when the neutron generator, the neutron source, and the detection system were raised together above the ground.

#### Discussion

To assess properly the soil volume sampled by an INS device is of critical importance for reporting absolute results of carbon measurements. The variability of this volume with changes in the soil conditions, in particular when scanning the soil, needs also to be addressed, although, it is believed that this effects will be small. The final sampled volume depends on the irradiated volume and the fraction of the irradiated volume seen by the detection system. Thus the number of detectors and their configuration will play a central role in defining the sampled volume. In the present work we analyzed only the irradiated volume that at isoflux level of 10% yielded a volume of about 277 1 (~9.8 ft<sup>3</sup>) or assuming bulk soil density of 1.5 g/cm<sup>3</sup> a mass of about 416 kg (~800 lb). Selection of the 10% level is very realistic and practical one that might be implemented in the future considerations when evaluating the final volume. The other volumes summarized in Table 1, were evaluated for a point source at 30 cm (1 ft) above the ground. It was shown IN fig. 1 that increasing the distance between the source and the ground decreased the neutron flux, however, at the same time it provided a more uniform, a smaller gradient, of the neutron flux in the soil, Fig. 2 thus improving the overall response of the system as shown by the 3D distributions in Figs. 3 and 4. The iso-counters used for calculating the volumes in Table 1 are shown in Figs 5 and 6. The reduction in the neutron flux gradient in soil is partially attributable to the flattening of the surface flux shown in Fig. 7 and also to the in-scattering from parallel wider beams, which approximate isotropic beam coming from large distances, shown in Fig. 8. The carbon yield is also affected by the neutron energy spectrum that changes with depth. Fig. 9. This additional complication will have to be considered carefully when evaluating the detectors configuration and the resulting counting efficiency. Finally, the arguments discussed here were demonstrated experimentally when the source and the detection system were raised together above the ground and the net carbon signal was monitored versus height. The net carbon signal maximized at about 25 to 30 cm above the ground confirming the fact that there is optimal height above, which the carbon signal decreases.

In summary, the calculations demonstrate that the irradiated volumes in INS are large that would result in large final samples seen by this method. Furthermore, MCNP simulations allow

isolating specific processes for better understanding of the neutron-gamma transport and based on the flux contours spacing of about 250 cm between the scans is required to have a uniform coverage of large areas.

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Table 1. Soil volumes and masses defined by the isofluxes for two neutron generator (NG) neutron source positions. The underlined values are the most plausible.

Isoflux	Volume (l)	Volume (l)	Mass (kg)	Mass (kg)
Level (%)	Ng @ 5 cm	Ng @ 30 cm	Ng @ 5 cm	Ng @ 30 cm
90	0.009	0.338	0.013	0.507
50	0.118	11.684	0.177	17.524
10	3.461	<u>277.430</u>	5.191	416.415
1.0	75.653	1,777.510	103.478	2,666.325
0.1	645.486		968.229	

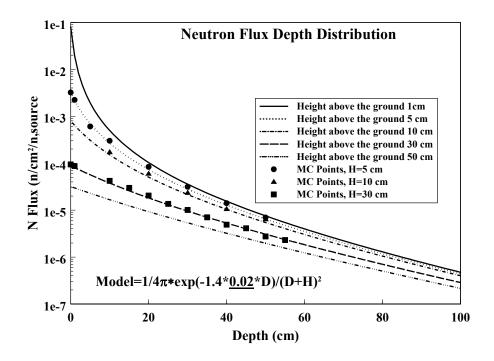


Figure 1. Neutron flux distributions in soil calculated for various heights of the neutron source above the ground using Monte Carlo, discrete points. Lines represent the model with the underlined parameter fitted.

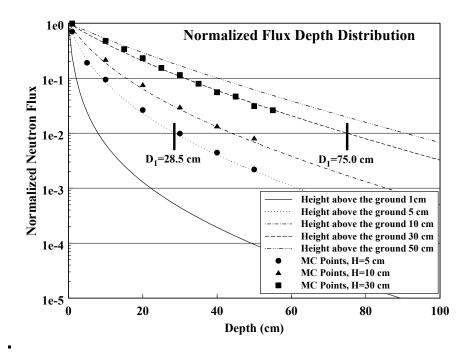


Figure 2. Normalized neutron flux in soil from Fig.1 and one percent levels of neutron flux marked by  $D_1$ .

# Normalized Neutron Flux Distribution Source 5 cm Above the Ground, Norm=293910, 108 Histories

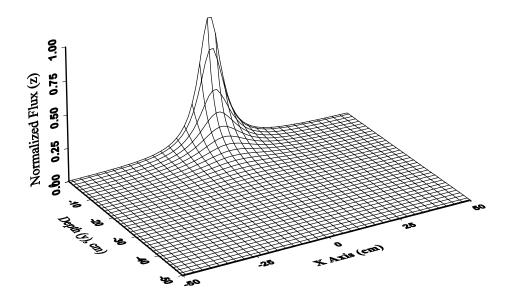


Figure 3. Three-dimensional display of the relative neutron flux in soil from a point source position 5 cm above the ground. The neutron flux is normalized at (0,0).

# **Normalized Neutron Flux Distribution**

Source 30 cm Above the Ground, Norm=8842, 108 Histories

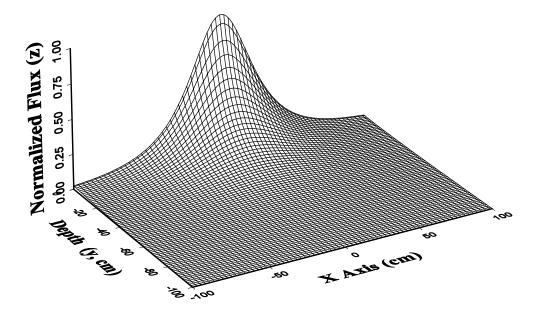


Figure 4. Three-dimensional display of the relative neutron flux in soil from a point source position 30 cm above the ground. The neutron flux is normalized at (0,0).

# Iso-Contours at 0.1, 1.0, 10, 50, 90% Levels Neutron Source 5 cm Above the Ground

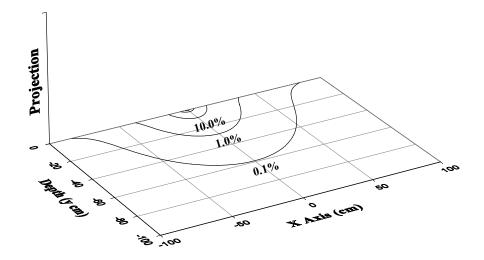


Figure 5. Isoflux contour lines at 0.1, 1.0, 10.0, 50, 90 percent levels for a source 5 cm above the ground.

# Iso-Contours at 0.1, 1.0, 10, 50, 90% Levels Neutron Source 30 cm Above the Ground

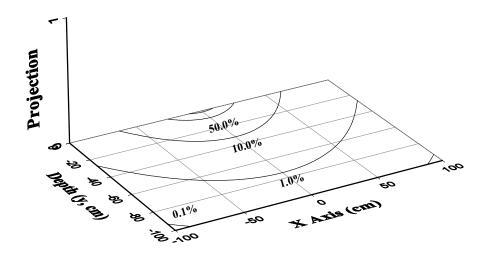


Figure 6 Isoflux contour lines at 0.1, 1.0, 10.0, 50, 90 percent levels for a source 30 cm above the ground.

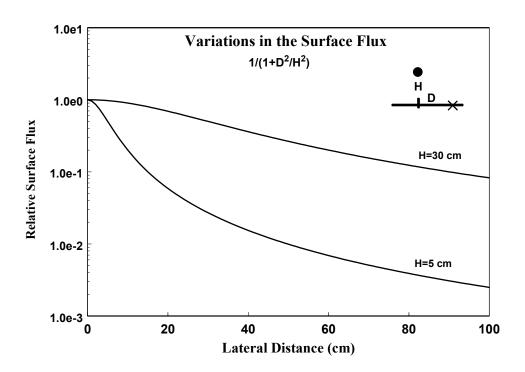


Figure 7. Normalized surface flux for two source positions above the ground.

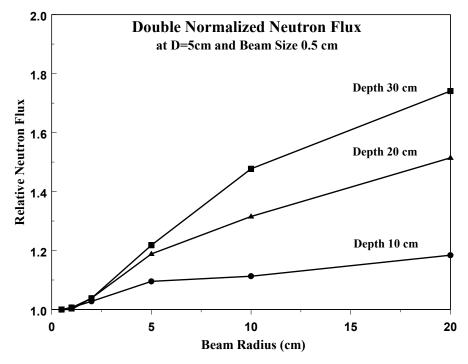


Figure 8. Relative effect of the parallel beam diameter on the neutron flux at fixed locations in the soil.

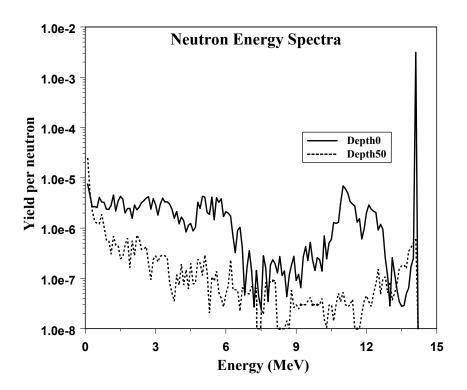


Figure 9. Neutron energy spectra at 0 and 50 cm deep resulting from a point source.

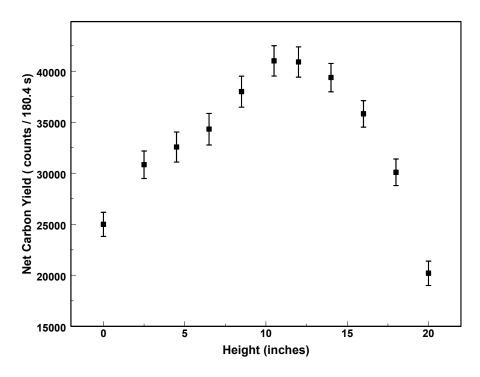


Figure 10. Net carbon yield as a function of the source and detection system height above the ground.